CCSF PHYC 4D Lecture Notes

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Chapter 4b
The Wavelike Properties of Particles (Part 2)

Wave packets and uncertainty relations

- Consider a classical wave of a single wave number k ($\lambda = 2\pi/k$):

$$y(x) = A\cos(kx)$$

  This wave extends throughout all of space. The wave number k is precisely known, but the position of the wave x is completely unknown.

- If we try to localize the classical wave by multiplying the cosine function by a localized function, such as a Gaussian, we can obtain a wave packet ([Ch4b:p1]).

$$y(x) = Ae^{-\alpha(x-x_0)^2}\cos(kx)$$

- It turns out that such a wave packet cannot be regarded as having a single wave number (or equivalently, a single wavelength), but instead must be a superposition of many waves with *different* wave numbers. As we will see, the more localized the wave packet, the larger the range of k values required to generate it.

- There is an uncertainty relationship between x and k given by

$$(\Delta x)(\Delta k) \geq \tfrac{1}{2}$$

  Equality occurs specifically for a Gaussian wave packet. In general, other wave packets will obey the strict inequality. It is impossible to obtain a product of uncertainties less than $\frac{1}{2}$.

- One obtains a similar result between t and ω when the time-dependence of the wave is introduced:

$$(\Delta t)(\Delta \omega) \geq \tfrac{1}{2}$$

  Again, equality occurs for the Gaussian.

- The uncertainty relations involving energy and momentum can be obtained from these by using the de Broglie relations:

$$(\Delta x)(\Delta p) = (\Delta x)\hbar(\Delta k) \geq \tfrac{1}{2}\hbar$$

$$(\Delta t)(\Delta E) = (\Delta t)\hbar(\Delta \omega) \geq \tfrac{1}{2}\hbar$$

Superposition of waves: beats

- Suppose we add together two waves with different wave numbers ([Ch4b:p2]):

$$k_1 = k - \tfrac{1}{2}\Delta k \qquad k_2 = k + \tfrac{1}{2}\Delta k$$

  to get

$$y(x) = \tfrac{1}{2}A\cos(k_1 x) + \tfrac{1}{2}A\cos(k_2 x)$$

- After substitution and trig identities, one gets

$$\begin{aligned} y(x) &= \tfrac{1}{2}A\cos(kx - \tfrac{1}{2}\Delta k\, x) + \tfrac{1}{2}A\cos(kx + \tfrac{1}{2}\Delta k\, x) \\ &= \tfrac{1}{2}A\Big(\cos(kx)\cos(\tfrac{1}{2}\Delta k\, x) + \sin(kx)\sin(\tfrac{1}{2}\Delta k\, x) + \\ &\qquad \cos(kx)\cos(\tfrac{1}{2}\Delta k\, x) - \sin(kx)\sin(\tfrac{1}{2}\Delta k\, x)\Big) \\ &= A\cos(\tfrac{1}{2}\Delta k\, x)\cos(kx) \end{aligned}$$

  The $A\cos(\frac{1}{2}\Delta k\, x)$ prefactor represents the slowly varying "beat envelope". The wave itself oscillates quickly between $\pm A\cos(\frac{1}{2}\Delta k\, x)$.

- Nodes in the beat envelope occur at x_n, where

$$\tfrac{1}{2}\Delta k\, x_n = \pi/2 + n\pi$$

  Separation between adjacent nodes ($\Delta x = x_{n+1} - x_n$) satisfies the "uncertainty relation"

$$\Delta k \Delta x = 2\pi$$

  Note that the larger the separation of wave numbers, the shorter the beat envelope is.

- Does Δx above really represent the uncertainty in x? Is the wave really contained mostly (if not entirely) within a finite region of length Δx? No. The beat pattern repeats itself over and over again. There is some information gained about position, but not very much. The reason is because we did not make the best use of the range of values of k. We only included two wave numbers.

Representing waves using complex numbers

- When dealing with waves, it is often convenient to express them as the real part of a complex wave ($y(x) = \Re(y_c(x))$), expressed in terms of exponentials using the Euler relationship

$$e^{i\phi} = \cos\phi + i\sin\phi$$

Superposition calculations would then use identities involving exponentials (most notably: $e^{x+y} = e^x e^y$) rather than identities among the trig functions, and are often easier to perform.

- A wave with a single wave number k would be represented by an exponential

$$y_c(x) = Ae^{ikx}$$

Note that $y(x) = \Re(y_c(x)) = A\cos(kx)$, as we had before.

- Actually, a more general wave would involve a phase shift

$$y(x) = A\cos(kx + \phi)$$

and could be expressed as the real part of

$$y_c(x) = Ae^{i(kx+\phi)} = (Ae^{i\phi})e^{ikx} = A_c e^{ikx}$$

where $A_c = Ae^{i\phi}$ is the complex amplitude of the wave. The complex amplitude represents both the amplitude of the actual wave (A) *and* its phase shift ϕ, all in one complex number.

- The beat calculation in the previous section can now be carried out using exponentials:

$$\begin{aligned} y_c(x) &= y_{c1}(x) + y_{c2}(x) \\ &= \tfrac{1}{2}Ae^{ik_1x} + \tfrac{1}{2}Ae^{ik_2x} \\ &= \tfrac{1}{2}A\left(e^{i(kx-\frac{1}{2}\Delta k\, x)} + e^{i(kx+\frac{1}{2}\Delta k\, x)}\right) \\ &= A\,\frac{e^{-i\frac{1}{2}\Delta k\, x} + e^{i\frac{1}{2}\Delta k\, x}}{2}\, e^{ikx} \\ &= A\cos(\tfrac{1}{2}\Delta k\, x)e^{ikx} \end{aligned}$$

Here we used the identities:

$$\cos\phi = \frac{e^{i\phi} + e^{-i\phi}}{2} \qquad \sin\phi = \frac{e^{i\phi} - e^{-i\phi}}{2i}$$

Taking the real part of $y_c(x)$ converts the e^{ikx} oscillation into the $\cos(kx)$ that we obtained in the last section.

- Perhaps you feel that using complex numbers is more trouble than it is worth. After all, the trig identities involved in the beat calculation in the last section were not that bad to begin with. However, in the next section where we combine more waves, a calculation involving trig identities would be prohibitively complicated. That calculation is much more easily carried out with complex numbers.

Including more wave numbers

- Now consider the superposition of $N+1$ waves of equally spaced wave numbers
$$k_n = k - \tfrac{1}{2}\Delta k + n\delta k \qquad (0 \le n \le N)$$
all falling within the range $[k - \frac{1}{2}\Delta k, k + \frac{1}{2}\Delta k]$, with adjacent values of k_n separated by $\delta k = \Delta k/N$. The superposition itself can be written
$$y(x) = \sum_{n=0}^{N} \frac{A}{N+1} \cos(k_n x)$$

- This calculation is most easily done using complex numbers:
$$\begin{aligned}
y_c(x) &= \frac{A}{N+1} \sum_{n=0}^{N} e^{ik_n x} \\
&= \frac{A}{N+1} e^{i(k-\frac{1}{2}\Delta k)x} \sum_{n=0}^{N} \left(e^{i\delta k\,x}\right)^n \\
&= \frac{A}{N+1} e^{i(k-\frac{1}{2}\Delta k)x} \frac{\left(e^{i\delta k\,x}\right)^{N+1} - 1}{e^{i\delta k\,x} - 1} \\
&= \frac{A}{N+1} e^{ikx} e^{-i\frac{1}{2}N\delta k\,x} \frac{e^{i\frac{1}{2}(N+1)\delta k\,x}}{e^{i\frac{1}{2}\delta k\,x}} \frac{e^{i\frac{1}{2}(N+1)\delta k\,x} - e^{-i\frac{1}{2}(N+1)\delta k\,x}}{e^{i\frac{1}{2}\delta k\,x} - e^{-i\frac{1}{2}\delta k\,x}} \\
&= A \frac{\sin(\frac{1}{2}(N+1)\delta k\,x)}{(N+1)\sin(\frac{1}{2}\delta k\,x)} e^{ikx}
\end{aligned}$$
The actual wave is given by the real part of the complex wave:
$$y(x) = \Re(y_c(x)) = A\frac{\sin(\frac{1}{2}(N+1)\delta k\,x)}{(N+1)\sin(\frac{1}{2}\delta k\,x)} \cos(kx)$$

- The envelope function (everything that multiplies $\cos(kx)$) has a principle range surrounded by two nodes separated by Δx, where

$$\tfrac{1}{2}(N+1)\delta k \Delta x = 2\pi \qquad \Delta k \Delta x = \frac{4\pi N}{N+1}$$

(Note: the envelope does not vanish when $x = 0$ because the denominator also goes to zero). The numerator of this envelope function is periodic with period $\frac{1}{2}\Delta x$, but the denominator grows and fades over a much longer range of x, resulting in an envelope that tapers off substantially after the principle range. For large N, this wave is significantly more localized that with just 2 waves ([Ch4b:p3]).

- The wave is still not completely localized. After a much longer shift in x ($2\pi N/\Delta k$), the denominator approaches zero again, resulting in another localized wave packet. However, if one takes $N \to \infty$, this repeated wave packet never appears. The wave packet is truly localized.

- At the heart of the derivation above is the evaluation of the "geometric series"

$$\sum_{n=0}^{N} \left(e^{i\delta k\, x}\right)^n$$

This sum can be done in general

$$S = \sum_{n=0}^{N} r^n = \frac{r^{N+1} - 1}{r - 1}$$

This result can be proven by multiplying out $(r-1)S$ and noting that most of the terms cancel out.

Continuous distribution of wave numbers: wave packets

- The limit $N \to \infty$ occurs when we consider a *continuous* distribution of wave numbers.

- In general, a wave packet is a superposition of waves over a continuous distribution of wave numbers, as follows

$$y(x) = \int_0^\infty A(k) \cos(kx)\, dk$$

or, equivalently, as the real part of

$$y_c(x) = \int_{-\infty}^{\infty} A(k) e^{ikx}\, dk$$

The second form is often easier to use and is the form we will use. Including negative values of k and allowing complex amplitudes $A(k)$ allows us to include sines as well as cosines, and allows us to handles cases where the wave is truly complex (such as the wavefunctions of quantum mechanics).

- Example #1: Constant amplitude over a finite range Δk.

$$A(k) = \begin{cases} A/\Delta k & \text{if } k_0 - \frac{1}{2}\Delta k \le k \le k_0 + \frac{1}{2}\Delta k \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned} y_c(x) &= \int_{-\infty}^{\infty} A(k) e^{ikx}\, dk = \int_{k_0-\frac{1}{2}\Delta k}^{k_0+\frac{1}{2}\Delta k} (A/\Delta k) e^{ikx}\, dk \\ &= \frac{A}{\Delta k} \frac{e^{ikx}}{ix}\bigg|_{k_0-\frac{1}{2}\Delta k}^{k_0+\frac{1}{2}\Delta k} = A \frac{\sin(\frac{1}{2}\Delta k\, x)}{\frac{1}{2}\Delta k\, x} e^{ik_0 x} \end{aligned}$$

Plugging in $\delta k = \Delta k/N$ in the formula for finite N and using the small angle approximation $\sin(x) \approx x$ for the denominator, one can show that this result is the same as the $N \to \infty$ limit of the finite N case.

- The envelope function is zero when $(\frac{1}{2}\Delta k)x = n\pi$ (except $n = 0$ when the denominator also vanishes), so the principle range of this wave packet is confined to a space Δx where $\Delta k \Delta x = 4\pi$. Unlike the finite case, the principle range never repeats.

- Example #2: Gaussian wave packet. The Gaussian probability distribution centered around x_0 with standard deviation σ is given by

$$P(x) = P_0 \exp\left(-\frac{(x - x_0)^2}{2\sigma^2}\right)$$

where P_0 is a suitably defined normalization coefficient (it happens to be $1/(\sigma\sqrt{2\pi})$, but we won't worry about that now).

- A useful Gaussian integral:

$$\int_{-\infty}^{\infty} \exp(-\alpha(t - t_0)^2 + \beta t)\, dt = \sqrt{\frac{\pi}{\alpha}} \exp\left(\beta x_0 + \frac{\beta^2}{4\alpha}\right)$$

where α, β, and t_0 are complex numbers with $\Re(\alpha) > 0$ (and $\Re(\sqrt{\alpha}) > 0$).

- Since probabilities are proportional to amplitude *squared*, it will be appropriate to take as our Gaussian wave packet the following distribution of wave numbers (note the $4\sigma_k^2$ instead of $2\sigma_k^2$):

$$A(k) = A\exp\left(-\frac{(k-k_0)^2}{4\sigma_k^2}\right)$$

- Now plug in ($t \to k$, $\alpha = 1/(4\sigma_k^2)$, and $\beta = ix$):

$$\begin{aligned} y_c(x) &= \int_{-\infty}^{\infty} A(k)e^{ikx}\,dk = \int_{-\infty}^{\infty} A\exp\left(-\frac{(k-k_0)^2}{4\sigma_k^2} + ikx\right) dk \\ &= A\sqrt{4\pi\sigma_k^2}\exp\left((ix)k_0 + \frac{(ix)^2}{4/(4\sigma_k^2)}\right) \\ &= A\sigma_k\sqrt{4\pi}\exp(-x^2\sigma_k^2)e^{ik_0x} \end{aligned}$$

- This is a Gaussian wave packet centered at $x = 0$ with a standard deviation of σ_x, where $1/(4\sigma_x^2) = \sigma_k^2$. This can be rearranged as follows:

$$\sigma_x\sigma_k = \tfrac{1}{2}$$

  This is a true uncertainty relation (the σ's actually represent uncertainties, and are not just estimates). The Gaussian wave packet provides the minimum possible value of $\sigma_x\sigma_k$.

- To get a Gaussian wave packet centered at x_0 instead of zero, simply replace $A(k)$ as follows:

$$A(k) \to A(k)e^{-ikx_0}$$

  Plugging into the expression for $y_c(x)$ gives a factor of $e^{ik(x-x_0)}$ in place of e^{ikx}, and thus results in $x \to x - x_0$.

The Fourier transform

- We have seen how a wave packet can be constructed from an amplitude function $A(k)$ by
$$y_c(x) = \int_{-\infty}^{\infty} A(k)e^{ikx}\,dk$$
Can we go the other way? Can any function $y_c(x)$ be constructed from a superposition of waves using some amplitude function $A(k)$?

- Yes (after making some continuity assumptions).
$$\begin{aligned}
\Gamma(k_0) &= \int_{-B}^{B} y_c(x)e^{-ik_0x}\,dx \\
&= \int_{-B}^{B} dx\, e^{-ik_0x} \int_{-\infty}^{\infty} dk\, A(k)e^{ikx} \\
&= \int_{-\infty}^{\infty} dk\, A(k) \int_{-B}^{B} dx\, e^{i(k-k_0)x} \\
&= \int_{-\infty}^{\infty} dk\, A(k) \left.\frac{e^{i(k-k_0)x}}{i(k-k_0)}\right|_{-B}^{B} \\
&= \int_{-\infty}^{\infty} dk\, A(k)\frac{2\sin((k-k_0)B)}{k-k_0}
\end{aligned}$$
Now substitude $u = (k-k_0)B$ ($k = k_0 + u/B$) and take $B \to \infty$.
$$\begin{aligned}
\Gamma(k_0) &= 2\int_{-\infty}^{\infty} \frac{du}{B}\, A(k_0 + u/B)\frac{\sin(u)}{u/B} \\
&= 2A(k_0)\int_{-\infty}^{\infty} \frac{\sin(u)}{u}\,du \\
&= 2\pi A(k_0)
\end{aligned}$$
It follows that
$$A(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} y_c(x)e^{-ikx}\,dx$$

- $A(k)$ defined above is called the Fourier transform of $y_c(x)$. Fourier transforms play an important role in wave analysis. It shows that any wave packet can be expressed as a superposition of waves of different wave numbers.

- A general function $y_c(x)$ defined over an unbounded interval requires a superposition over a continuum of wave numbers. On the other hand, a function $y_c(x)$ defined only over a finite interval of length L (or if $y_c(x)$ is

periodic with period L) can be obtained from a discrete superposition:

$$y_c(x) = \sum_{n=-\infty}^{\infty} A_n e^{ik_n x}$$

where $k_n = nk_1 = 2\pi n/L$. These wave numbers correspond to wavelengths $\lambda_n = L/n$.

- This sum can also be written in terms of sines and cosines:

$$y_c(x) = \tfrac{1}{2}B_0 + \sum_{n=1}^{\infty} \left(B_n \cos(k_n x) + C_n \sin(k_n x)\right)$$

but the exponential form is often more convenient.

- The coefficients can all be computed from $y_c(x)$:

$$\begin{aligned} A_n &= \frac{1}{L}\int_a^b y_c(x) e^{-ik_n x}\,dx \qquad (-\infty < n < \infty) \\ B_n &= A_n + A_{-n} = \frac{2}{L}\int_a^b y_c(x)\cos(k_n x)\,dx \qquad (0 \le n < \infty) \\ C_n &= i(A_n - A_{-n}) = \frac{2}{L}\int_a^b y_c(x)\sin(k_n x)\,dx \qquad (0 < n < \infty) \end{aligned}$$

where $y_c(x)$ is defined over the range $[a, b]$ with $L = b - a$.

- Note that the separation between values of k ($\Delta k = k_{n+1} - k_n = 2\pi/L$) is inversely related to L. The longer the interval in x, the smaller the separation between k values. As $L \to \infty$, $\Delta k \to 0$, which leads us back to the continuous distribution of k values.

Time dependence

- The waves considered above were all snapshots at some fixed time (e.g., $t = 0$). If we instead fix x (say, at $x = 0$) and consider the time-dependence of the wave at that fixed position (or else consider an oscillation which has no spatial dependence), we obtain

$$y(t) = A\cos(-\omega t)$$

which is the real part of

$$y_c(t) = Ae^{-i\omega t}$$

Substituting $x \to t$ and $k \to -\omega$, everything we have discussed so far applies equally well to the time-dependence of waves and oscillations. In particular, an oscillation that is confined to a finite time interval Δt must be constructed from a superposition of oscillations of different (angular) frequencies, which must obey the uncertainty relation

$$\Delta t \Delta \omega \geq \tfrac{1}{2}$$

- Now consider the full space-time dependence of a wave. For a single wave number, the wave takes on the form

$$y(x,t) = A\cos(kx - \omega t)$$

which is the real part of

$$y_c(x,t) = Ae^{i(kx-\omega t)}$$

Wave fronts are defined by $\cos(kx-\omega t) = +1$. If a particular wave front (characterized by an integer n, so that $kx - \omega t = 2\pi n$) moves from x_1 to x_2 during the time interval from t_1 to t_2, then

$$kx_1 - \omega t_1 = 2\pi n = kx_2 - \omega t_2$$

This wave front moves with the wave's *phase* velocity, v_p, given by

$$v_p = \frac{x_2 - x_1}{t_2 - t_1} = \frac{\omega}{k}$$

The wave can be expressed in terms of this phase velocity:

$$y_c(x,t) = Ae^{ik(x-v_p t)} = f(x - v_p t)$$

which is the general form for any disturbance that travels with velocity v_p through space.

- Now consider a superposition of such waves

$$y_c(x,t) = \int_{=\infty}^{\infty} A(k)e^{i(kx-\omega t)}\, dk$$

The behavior of the wave packet over time will depend specifically on how ω depends on k, which depends on the type of wave. The equation relating ω and k is called a *dispersion relationship*.

- Suppose $v_p = \omega/k$ is independent of k, so that

$$\omega = v_p k \qquad v_p \text{ is a constant}$$

Then

$$\begin{aligned} y_c(x,t) &= \int_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)}\, dk \\ &= \int_{-\infty}^{\infty} A(k) e^{ik(x-v_p t)}\, dk \\ &= f(x - v_p t) \end{aligned}$$

where

$$f(x') = \int_{-\infty}^{\infty} A(k) e^{ikx'}\, dk$$

is the wave packet at $x = x'$ and $t = 0$. Evidently the wave packet moves through space with its center travelling with velocity v_p, but the shape of the wave packet is otherwise unchanged. This makes sense, since each component wave travels with the same wave velocity. Waves obeying a simple linear relationship $\omega = v_p k$ are called *non-dispersive* for this reason.

- Now suppose the relationship between ω and k is more complicated, so that v_p depends on k. In this case, we can't simply substitute $x' = x - v_p t$ in the equation above and rewrite the wave packet in the form $f(x - v_p t)$ (the x' will depend on k). The wave packet will move with a different velocity and, in general, change shape over time. How exactly that happens depends on the details of the dispersion relation and the amplitude function $A(k)$.

- Suppose we perform a Taylor series expansion in $\omega(k)$ out to first order:

$$\omega \approx \omega_0 + v_g(k - k_0)$$

where $v_g = d\omega/dk|_{k=k_0}$. v_g has units of velocity and is called the *group* velocity, for reasons that will become clear in a moment. Suppose that this approximation remains a good one for all values of k where $A(k)$ is significant. Then

$$\begin{aligned} y_c(x,t) &= \int_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)}\, dk \\ &= \int_{-\infty}^{\infty} A(k) e^{i(kx-\omega_0 t - v_g k t + v_g k_0 t)}\, dk \end{aligned}$$

$$\begin{aligned} &= \int_{-\infty}^{\infty} A(k) e^{ik(x-v_g t)} e^{i(k_0 v_g - \omega_0)t}\, dk \\ &= f(x - v_g t) e^{ik_0(v_g - v_p)t} \end{aligned}$$

where $f(x')$, as before, represents the wave packet at $t = 0$. In this case, the center of the wave packet does not move with the phase velocity v_p, but instead moves with the group velocity v_g. The exponential that follows $f(x - v_g t)$ corrects the *phase* (but not the amplitude) of the wave for the fact that wave fronts continue moving with velocity v_p. The result is a wave packet that travels with velocity v_g as the wave fronts of the constituent waves continue travelling with velocity v_p.

- Note: if $\omega = v_p k$, where v_p is actually constant, then

  $$v_g = d\omega/dk = v_p$$

  and this result reduces to the earlier result.

- If the approximation

  $$\omega \approx \omega_{\text{approx}} = \omega_0 + v_g(k - k_0) \qquad v_g \text{ constant}$$

  is not a very good one (or if one waits long enough), then the wave packet will change shape. What typically happens is that the wave packet starts out narrow (small Δx), but then disperses over time as the constituent waves travel with different velocities. It is interesting that the wider the wave packet is to begin with, the less dispersion one is likely to see because the range of k's that make up the wave packet can be quite narrow (large Δx implies small Δk). Conversely, a wave packet that starts out very narrow (small Δx) will grow rapidly since such a wave packet must necessarily involve a wide range of k values. Physically, this makes sense in light of the uncertainty relations: if a particle is initially confined to a tight region, the uncertainty in its position will grow rapidly as the particle leaves the confined region with a poorly defined momentum.

- Note: If v_p increases with increasing k, then $v_g > v_p$. If v_p decreases with increasing k, then $v_g < v_p$, and may even point in the opposite direction. This can be explained by following the beat pattern for the superposition of two waves k_1 and k_2 travelling with different phase velocities. Diagrams in [Ch4b:p5] illustrate this.

- Technical note: to better understand the conditions under which the approximation

$$\omega \approx \omega_0 + v_g(k - k_0) \qquad v_g \text{ constant}$$

is a good one, we can write

$$\omega = \omega_0 + v_g(k - k_0) + \delta\omega$$

where $\delta\omega$ represents the deviation between ω and its approximate value (it is a function of k). Substituting this into the wave packet formula yields

$$\begin{aligned} y_c(x,t) &= \int_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)}\, dk \\ &= \int_{-\infty}^{\infty} A(k) e^{ik(x-v_g t)} e^{-i\delta\omega\, t} e^{i(k_0 v_g - \omega_0)t}\, dk \end{aligned}$$

The approximation involves setting the exponential factor $e^{-i\delta\omega\, t}$ equal to 1. This is a reasonable approximation as long as $|\delta\omega\, t| \ll 2\pi$ for all values of k where $A(k)$ is significant. Note that this approximation will eventually break down over time, unless $\delta\omega = 0$ exactly for all relevant values of k.

The wavefunction

- Recall that the intensity of a wave disturbance given by $y(x,t)$ is proportional to $|y(x,t)|^2$. When we consider a *probability wave*, that intensity is directly related to the probability of finding a particle in a given location.
- In Part 1 of Chapter 4, we talked about how particle waves are probability waves. For simple particles confined to one dimension, the particle wave is described by a *wave function* $\psi(x,t)$, such that the probability of finding the particle in the interval $[x, x+dx]$ at time t is given by

$$P(x,t)\, dx = |\psi(x,t)|^2\, dx$$

- Note that when computing $|y(x,t)|^2$ for a wave, we must carefully distinguish between $y(x,t)$ itself (which may be expressed in terms of cosine and sine functions), and $y_c(x,t)$, which includes an imaginary part. There is a significant difference between $|y(x,t)|^2$ and $|y_c(x,t)|^2$. For traditional waves which are manifestly real-valued, the intensity is proportional to $|y(x,t)|^2$, not $|y_c(x,t)|^2$.

- With that in mind, consider a particle moving in one dimension with momentum p and energy E. According to de Broglie, this particle has wave number k and angular frequency ω given by

$$p = \hbar k \qquad E = \hbar \omega$$

It would make sense that such a wave would be described by

$$\psi(x,t) \stackrel{?}{=} A\cos(kx - \omega t)$$

We might use

$$\psi_c(x,t) = Ae^{i(kx-\omega t)}$$

in wave-packet calculations for convenience, but when we compute probability densities, we might expect to have to take the real part of $\psi_c(x,t)$ to get $\psi(x,t)$ before squaring it (the fact that this is *not* the case will be discussed shortly).

- According to the uncertainty principle, a particle with a precisely known momentum and energy ($\Delta p = 0$, $\Delta E = 0$) must have a completely unknown position ($\Delta x = \infty$) and last forever ($\Delta t = \infty$). If we look at the probability distribution for such a wave

$$P(x,t)\,dx = |\psi(x,t)|^2\,dx \stackrel{?}{=} |A|^2\cos^2(kx-\omega t)\,dx$$

it is certainly the case that the wave is delocalized both in space and time. However, it appears that the probability density does depend on position and time ($\cos^2(kx - \omega t)$ oscillates between 0 and 1).

- In a different universe than our own, it might have happened to work out this way, but this oscillation in the probability density is not actually observed. Instead, a particle with definite momentum and energy is observed to have a *uniform* probability density throughout space: $|\psi(x,t)|^2$ is a *constant*, independent of both x and t.

- How do we reconcile this? By defining the wave function as a complex number

$$\psi(x,t) = Ae^{i(kx-\omega t)}$$

This is the reality of the wave function. It is *not* the real (or imaginary) part of anything. It is a complex number. That is the way it is. This leads to a constant probability density, as claimed

$$|\psi(x,t)|^2 = |Ae^{i(kx-\omega t)}|^2 = |A|^2$$

Note: $|e^{i\phi}| = |\cos\phi + i\sin\phi| = \sqrt{\cos^2\phi + \sin^2\phi} = 1$.

Wave-packet wave functions

- A wave packet can be constructed for wave functions in much the same way that we constructed them for general waves. These wave packets are appropriate for particles whose probability density is confined to a local region of space. The fact that a localized wave packet is a superposition of waves with different wave numbers is a reflection of the uncertainty principle.

$$(\Delta x)(\Delta p) = \hbar(\Delta x)(\Delta k) \geq \tfrac{1}{2}\hbar$$

- Some general things to notice as we revisit these wave packets:
  - The probability density is uniform for a single wave number — the oscillatory part does not contribute — but when two or more waves interfere, the relative phases of the interfering waves *do* matter.
  - The (time-independent) wave packets are, in general, of the form

$$\psi(x) = (\text{envelope function})e^{ik_0x}$$

    The overall oscillation part does not contribute to the probability density, but the envelope function, which results from the interference, does.
  - Once again, when we bring the time dependence back into the picture, the wave packet will travel with the group velocity $v_g = d\omega/dk$, and in general, may change shape (usually spreading out) over time.

- Beats (suppress time-dependence for now):

$$k_1 = k_0 - \tfrac{1}{2}\Delta k \qquad k_2 = k_0 + \tfrac{1}{2}\Delta k$$

$$\psi(x) = \tfrac{1}{2}Ae^{ik_1x} + \tfrac{1}{2}Ae^{ik_2x} = A\cos(\tfrac{1}{2}\Delta k\, x)e^{ik_0x}$$

$$P(x)\,dx = |\psi(x)|^2\,dx = |A|^2\cos^2(\tfrac{1}{2}\Delta k\, x)\,dx$$

- Special case: k and $-k$

$$\psi(x) = \tfrac{1}{2}Ae^{ikx} + \tfrac{1}{2}Ae^{i(-k)x} = A\cos(kx)$$

$$P(x)\,dx = |A|^2\cos^2(kx)\,dx$$

Evidently, the cosine we originally proposed for the wave function of definite momentum actually applies to a particle that is equally likely to be moving in either of two directions. The oscillatory behavior of $P(x)$ is due to the interference of the two probability waves. One needs to be careful, however, when reintroducing the time dependence. ω is always positive, so

$$\psi(x,t) = \tfrac{1}{2}Ae^{i(kx-\omega t)} + \tfrac{1}{2}Ae^{i(-kx-\omega t)} = A\cos(kx)e^{-i\omega t}$$

$$P(x,t)\,dx = |A|^2\cos^2(kx)\,dx$$

This is a standing wave pattern. The probability distribution does *not* shift over time.

- The continuous case:

$$\psi(x) = \int_{-\infty}^{\infty} A(k)e^{ikx}\,dk$$

For the uniform amplitude over a finite range Δk:

$$\psi(x) = A\frac{\sin(\frac{1}{2}\Delta k\,x)}{\frac{1}{2}\Delta k\,x}e^{ik_0x}$$

$$P(x) = |\psi(x)|^2 = |A|^2\left(\frac{\sin(\frac{1}{2}\Delta k\,x)}{\frac{1}{2}\Delta k\,x}\right)^2$$

For the Gaussian

$$A(k) = A\exp\left(-\frac{(k-k_0)^2}{4\sigma_k^2}\right)e^{-ikx_0}$$

we get

$$\psi(x) = A\sigma_k\sqrt{4\pi}\exp\left(-\frac{(x-x_0)^2}{4\sigma_x^2}\right)e^{ik_0x}$$

$$P(x) = 4\pi\sigma_k^2|A|^2\exp\left(-\frac{(x-x_0)^2}{2\sigma_x^2}\right)$$

where $\sigma_x\sigma_k = \frac{1}{2}$.

- Including time dependence:

$$\psi(x,t) = \int_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)}\, dk$$

If we define

$$f(x') = \int_{-\infty}^{\infty} A(k) e^{ikx'}\, dk$$

to be the wave packet at $x = x'$ and $t = 0$, and make the approximation

$$\omega = \omega_0 + v_g(k - k_0) \qquad v_g = d\omega/dk$$

then we get

$$\psi(x,t) = f(x - v_g t) e^{ik_0(v_g - v_p)t}$$

Again, this is a wave packet whose envelope travels at the group velocity v_g and whose constituent waves within the envelope travel at the phase velocity v_p (the exponential post-factor corrects for this). The overall phase factors, however, do not contribute to the probability:

$$P(x,t) = |\psi(x,t)|^2 = |f(x - v_g t)|^2$$

The probability distribution travels with the group velocity. Over time, the approximation for ω breaks down and the wave packet changes shape (usually expanding in size over time).

- For a non-relativistic particle, $E = p^2/2m$. Substituting the de Broglie relations yields the dispersion relation

$$\omega = \hbar k^2/(2m)$$

The phase and group velocities are given by

$$v_p = \omega/k = \hbar k/(2m) = p/(2m) \qquad v_g = d\omega/dk = \hbar k/m = p/m$$

A classical particle can be modeled as a narrow wave packet defined over a narrow range of k values (the uncertainty principle is not very restrictive in the classical limit). That wave packet travels at the group velocity, which coincides with the classical velocity of the particle.

- For a relativistic particle,

$$E^2 = p^2c^2 + m^2c^4$$

Differentiating both side with respect to p yields

$$2EdE/dp = 2pc^2$$

The group velocity in this case is

$$v_g = d\omega/dk = dE/dp = pc^2/E = \gamma mvc^2/(\gamma mc^2) = v$$

Appendix: Time-dependent Gaussian wave packet with quadratic dispersion

- Consider a Gaussian amplitude function

$$A(k) = A \exp\left(-\frac{(k-k_0)^2}{4\sigma_k^2}\right) e^{-ikx_0}$$

The time-independent wave packet comes out to

$$\psi(x) = A\sigma_k\sqrt{4\pi}\exp\left(-\frac{(x-x_0)^2}{4\sigma_x^2}\right) e^{ik_0 x}$$

where $\sigma_x\sigma_k = \frac{1}{2}$.

- Now consider the full time-dependent wave packet with a quadratic dispersion relation $\omega = Ck^2$. The phase and group velocities are given by

$$v_g = d\omega/dk|_{k=k_0} = 2Ck_0 \qquad v_p = \omega/k|_{k=k_0} = Ck_0 = \tfrac{1}{2}v_g$$

The dispersion relation can be expressed in terms of the group velocity

$$\omega = \frac{v_g}{2k_0}k^2$$

This time we make no approximations.

- Preparitory algebra:

$$k^2 = (k-k_0)^2 + 2kk_0 - k_0^2$$
$$\omega t = \frac{v_g t}{2k_0}(k-k_0)^2 + kv_g t - \tfrac{1}{2}k_0 v_g t$$

- Now plug in:

$$\begin{aligned}
\psi(x,t) &= \int_{-\infty}^{\infty} A(k)e^{i(kx-\omega t)}\,dk \\
&= \int_{-\infty}^{\infty} A\exp\left(-\frac{(k-k_0)^2}{4\sigma_k^2} - ikx_0 + ikx - i\frac{v_g t}{2k_0}(k-k_0)^2 - ikv_g t + \tfrac{1}{2}ik_0 v_g t\right)dk \\
&= \int_{-\infty}^{\infty} A\exp\left(-\left(\frac{1}{4\sigma_k^2} + i\frac{v_g t}{2k_0}\right)(k-k_0)^2 + ik(x-x_0-v_g t) + \tfrac{1}{2}ik_0 v_g t\right)dk
\end{aligned}$$

- A useful Gaussian integral (repeat from before):

$$\int_{-\infty}^{\infty}\exp(-\alpha(x-x_0)^2 + \beta x)\,dx = \sqrt{\frac{\pi}{\alpha}}\exp\left(\beta x_0 + \frac{\beta^2}{4\alpha}\right)$$

Define

$$\alpha = \frac{1}{4\sigma_k^2} + i\frac{v_g t}{2k_0} = \frac{1+it/\tau}{4\sigma_k^2} \qquad \tau = \frac{2k_0}{4\sigma_k^2 v_g}$$

and

$$\beta = i(x - x_0 - v_g t)$$

Note that

$$\frac{1}{\alpha} = \frac{4\sigma_k^2}{1 + it/\tau} = \frac{4\sigma_k^2(1 - it/\tau)}{1 + t^2/\tau^2} = \frac{1 - it/\tau}{\sigma_x^2}$$

where

$$\sigma_x \sigma_k = \tfrac{1}{2}\sqrt{1 + t^2/\tau^2}$$

- Continuing the calculation:

$$\begin{aligned}
\psi(x,t) &= \int_{-\infty}^{\infty} A \exp(-\alpha(k - k_0)^2 + \beta k + \tfrac{1}{2} i k_0 v_g t)\, dk \\
&= A\sqrt{\frac{\pi}{\alpha}} \exp\left(\beta k_0 + \frac{\beta^2}{4\alpha} + \tfrac{1}{2} i k_0 v_g t\right) \\
&= \frac{A\sqrt{\pi(1 - it/\tau)}}{\sigma_x} \exp\left(i k_0 (x - x_0 - v_g t + \tfrac{1}{2} v_g t) - \frac{(x - x_0 - v_g t)^2}{4\sigma_x^2}(1 - it/\tau)\right) \\
&= \frac{A\sqrt{\pi(1 - it/\tau)}}{\sigma_x} \exp\left(i k_0 (x - x_0 - v_p t) + i\frac{(x - x_0 - v_g t)^2 t/\tau}{4\sigma_x^2} - \frac{(x - x_0 - v_g t)^2}{4\sigma_x^2}\right)
\end{aligned}$$

- The result is a Gaussian wave packet of width σ_x where

$$\sigma_x \sigma_k = \tfrac{1}{2}\sqrt{1 + t^2/\tau^2}$$

multiplied by a complicated phase factor. The probability density is much simpler because the phase factor doesn't contribute:

$$P(x,t) = |\psi(x,t)|^2 = \frac{|A|^2 \pi \sqrt{1 + t^2/\tau^2}}{\sigma_x^2} \exp\left(-\frac{(x - x_0 - v_g t)^2}{2\sigma_x^2}\right)$$

This Gaussian wave packet expands over time by a factor of $\sqrt{1 + t^2/\tau^2}$. The parameter

$$\tau = \frac{k_0}{2\sigma_k^2 v_g}$$

defines a characteristic time scale over which this expansion occurs. When $t \ll \tau$, the expansion of the wave packet is minimal and the approximation

$$\omega \approx \omega_0 + v_g(k - k_0)$$

is more accurate. As $t \to \tau$, this approximation begins to break down. As σ_k is decreased, we expect the approximation for ω to improve. Indeed, τ increases when σ_k decreases, implying that it takes longer for the approximation to break down and the wave packet to expand.